

Quantum Critical Universality and Singular Corner Entanglement Entropy of Bilayer Heisenberg-Ising model

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We consider a bilayer quantum spin model with anisotropic intra-layer exchange couplings. By varying the anisotropy, the quantum critical phenomena changes from XY to Heisenberg to Ising universality class, with two, three and one modes respectively becoming gapless simultaneously. We use series expansion methods to calculate the second and third Renyi entanglement entropies when the system is bipartitioned into two parts. Leading area-law terms and subleading entropies associated with corners are separately calculated. We find clear evidence that the logarithmic singularity associated with the corners is universal in each class. Its coefficient along the Ising critical line is in excellent agreement with those obtained previously for the transverse-field Ising model. Our results provide strong evidence for the idea that the universal terms in the entanglement entropy provide an approximate measure of the low energy degrees of freedom in the system.

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In recent years, the studies of ground state phases of strongly interacting quantum many-body systems have been greatly informed and enriched by new ideas from quantum information theory[1–4]. Locality of ground state entanglement propagation embodied in the ubiquitous ‘area-law’ for entanglement entropy, allows for powerful new variational approaches[5–7] that have the potential to transform computational materials science. This has naturally led to great interest in understanding and quantifying the amount of quantum entanglement present in the true ground states of many-body systems.

Bipartite entanglement entropy in the ground states of systems with a gap in the excitation spectrum is known

to obey the area-law[3], that is, the leading term scales with the ‘area’ measuring the boundary between the bipartitioned subsystems. In addition, such systems may also contain quantifiable signatures of topological phases in the form of a long-range entanglement entropy that is unrelated to any boundary[8–11]. Gapless modes can create additional longer-range entanglement and indeed the study of entanglement properties can provide novel ways to decipher Goldstone modes associated with spontaneous symmetry breaking[12], study different quantum critical universality classes[13, 14], as well as the geometrical properties of fermi surfaces[15–20]. However, while the studies of universality in entanglement properties of one-dimensional systems is rather extensive[13, 21], quantitative studies in higher dimensional lattice models remain few and far between[22–26].

On approach to the critical point, the entanglement entropies contain both non-universal and universal singular pieces[4]. In particular, the corner entropy is expected to have a logarithmic singularity with a universal coefficient. Some universal singular terms may also provide connections to underlying quantum field theories and the stability of fixed points under renormalization[26–28]. In one dimensional models, the singularities in the entanglement entropy are known[13] to be related to the conformal anomaly c , and thus, naturally provide a connection to Zamolodchikov’s c -theorem[29] that posits that under renormalization systems flow towards smaller c -values. There have been many recent efforts to generalize Zamolodchikov’s c -theorem to higher dimensional systems and the entanglement entropy is central to such efforts[30]. In a very general sense, one expects the singularities in the entanglement entropy to provide a measure of low lying fluctuations or a count of degrees of freedom in the underlying continuum theory[27, 28]. Quantum field theory calculations are difficult and hence numerical approaches must play an essential role.

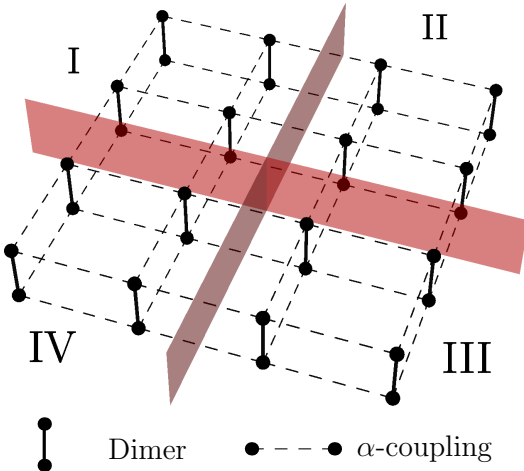


FIG. 1: A bilayer of quantum spins can be divided into half-bilayers or quarter-bilayers by a suitable choice of partitions. These can, in turn, be used to define the ‘area-law’ entanglement entropy (or the entanglement entropy per unit length of the boundary) and the corner entanglement entropy.

Here, we consider a bilayer consisting of two-planes of square-lattice of spins (see Fig. 1), with an anisotropic quantum Heisenberg model with Hamiltonian,

$$\mathcal{H} = \sum_{\langle i,j \rangle} (S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z) + \alpha \sum_{\langle\langle i,k \rangle\rangle} (S_i^x S_k^x + S_i^y S_k^y + \lambda S_i^z S_k^z), \quad (1)$$

where the first sum runs over pairs of spins between the two layers, while the second sum runs over the nearest-neighbor spins, within each layer. For $\alpha = 0$, this model is in the singlet phase, where each pair of inter-planar spins form a dimer. When α is large, the system goes from an XY order at small λ to Ising order at large λ . Right at $\lambda = 1$, full Heisenberg symmetry is realized and we have the well studied bilayer quantum Heisenberg model[26, 31–34]. In the singlet phase there are three single-particle excitations corresponding to $S^z = +1, 0$ and -1 respectively. As is evident from the symmetries of the model for $\lambda < 1$, the gap to $S^z = \pm 1$ modes closes first leading to XY order. For $\lambda > 1$, the gap to $S^z = 0$ mode closes first leading to Ising order. At $\lambda = 1$, all three modes remain exactly degenerate and the system has higher symmetry and Heisenberg universality. Thus, this model provides an elegant way to study the quantum-critical behavior and different universality classes and their crossovers in a two-dimensional quantum system.

To carry out our series expansions, we consider one value of the anisotropy λ at a time. We expand around the dimerized phase at $\alpha = 0$. To determine the critical coupling α_c at each λ , we calculate series for the staggered susceptibility and excitation gap. For $\lambda < 1$, we consider the staggered susceptibility to a field in the x -direction, and the $S^z = +1$ excitation gap. For $\lambda \geq 1$, we instead consider the staggered susceptibility to a field in the z -direction, and the $S^z = 0$ excitation gap.

We then calculate series expansions for the ‘area-law’ terms for the 2nd and 3rd Renyi entanglement entropies at various values of λ . To do this, we consider an $L \times L \times 2$ lattice with free boundary conditions. We bipartition the bilayer of spins into two equal size half-bilayers by one of the two dividers shown in Fig. 1. The left half-bilayer (regions I and IV) can be denoted A and the right half-bilayer (regions II and III) can be denoted B. The n th Renyi entropy is defined as

$$S_n(A) = \frac{1}{1-n} \ln \text{Tr}(\hat{\rho}_A^n), \quad (2)$$

where $\hat{\rho}_A = \text{Tr}_B |\Psi\rangle \langle \Psi|$ is the reduced density matrix for subsystem A. The length of the interface between A and B is given by L . We define the Renyi entanglement entropy per unit length of the interface, in the thermodynamic limit, as

$$s_n = \lim_{L \rightarrow \infty} S_n/L. \quad (3)$$

The quantities, s_n can be calculated, as a power series expansion in λ , by the linked cluster method[24, 35, 36].

The entropy due to the presence of a 90° corner in the boundary for the n th Renyi entropy, c_n , can also be isolated in our series expansions [24, 26]. This is done by calculating the entanglement entropy upon subdivision of the system by two perpendicular partitions (see Fig. 1), either into a quarter-bilayer (and its complement of 3-quarter bilayers) or into two half bilayers. The contributions from the linear boundaries can be cancelled out, by subtracting the entropies when the subsystem A is a half-bilayer from the case when it is a quarter bilayer [24]. This allows us to generate a separate series expansion for the corner entropy c_n .

All series coefficients are calculated up to α^{11} . A single calculation of this order can be completed within a day on a moderately powerful personal computer.

The series are analyzed using Pade and differential approximants[35, 36]. First we analyze the series for the susceptibility and gap series. These lead to the determination of the phase-boundary shown in Figure 2. The critical couplings α_c obtained from the susceptibility and gap series are consistent with each other. The critical exponents γ for the susceptibility divergence and ν for the gap closing (taking $z = 1$) are calculated and shown in Figure 3. Here, and throughout this paper, the error bars shown represent a spread in the different approximants and are not true statistical uncertainties. The results from epsilon expansion calculations, taken from the literature[37] are also shown. On the Ising side the exponents are within 1-2 percent of accepted values for the 3-dimensional Ising universality class, while on the XY side they are within 2-3 percent of accepted values for the 3-dimensional O(2) universality class[37]. Only at the Heisenberg point ($\lambda = 1$), the deviations are larger (approximately 6-7 percent for the susceptibility exponent γ). These are largely correlated with uncertainties in α_c , which varies sharply near the Heisenberg point. For example, the susceptibility series leads to estimates of $\alpha_c = 0.3982 \pm 0.0008$, with $\gamma = 1.51 \pm 0.02$. If we bias approximants to much more accurate values of the critical point from Quantum Monte Carlo simulations[31] $\alpha_c = 0.39651$, it leads to estimates for exponent of $\gamma = 1.43 \pm 0.02$, which are much closer to accepted values for the 3-dimensional classical O(3) universality class.

The area-law term in the entanglement entropy is known to have a weak singularity at the critical coupling. We simply used biased differential approximants, with the critical points α_c estimated from the susceptibility series, to obtain their values up to the critical coupling. The plots for s_2 and s_3 are shown in Figures 4 and 5 respectively. Our results should be highly accurate except possibly when one is within a few percent of the critical coupling. Two different approximants are plotted for s_2 for $\lambda = 1$ to show the expected deviations. The difference is barely visible in the plots. For the second

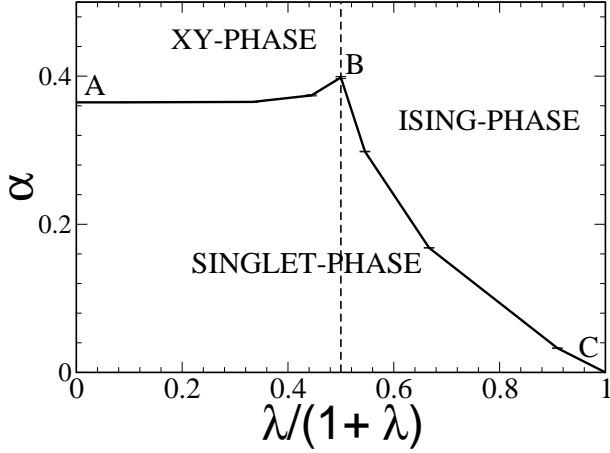


FIG. 2: The phase diagram of the model with the Singlet phase at small α and the ordered XY and Ising phases at large α . The dashed line represents the system with full Heisenberg symmetry. The critical point B has $O(3)$ universality class and separates $O(2)$ universality class along AB from Ising universality class along BC .

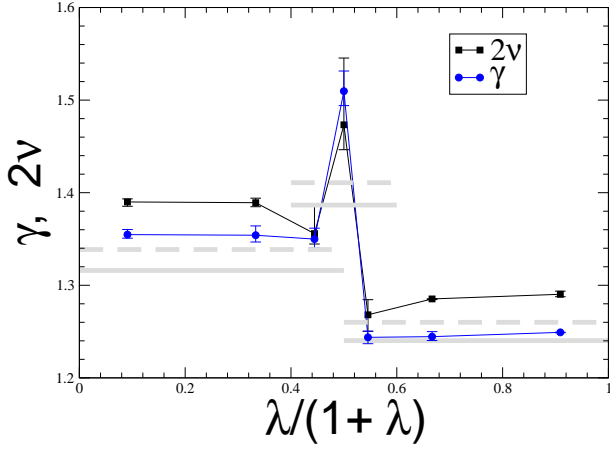


FIG. 3: Critical exponents γ and ν are shown for different values of the anisotropy parameter λ . Our results are consistent with constant values for the exponents in the XY and Ising regimes, with a larger exponent at the special Heisenberg symmetry case. The results from epsilon expansions[37] are shown as solid lines for γ and dashed lines for 2ν (On the right for Ising, on the left for XY and in the middle for classical Heisenberg universality class).

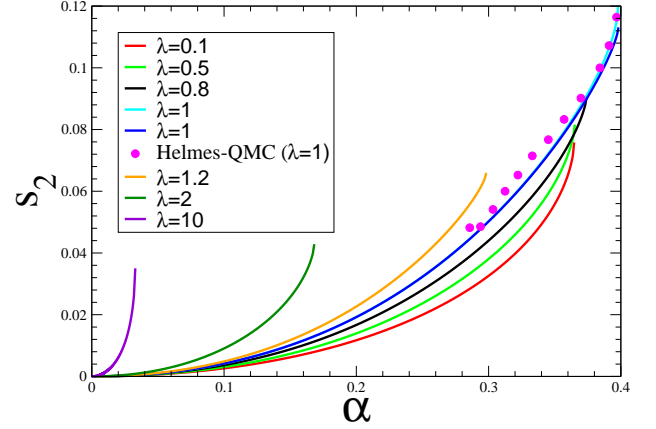


FIG. 4: Plots of the ‘Area-law’ or entanglement entropy per unit boundary length for the second Renyi entropy S_2 . Quantum Monte Carlo data from Helmes et al are shown by filled circles. For $\lambda = 1$ two approximants are shown for s_2/λ^2 series: a $[4,4]$ Pade approximant and a $[T = 0, M = 3, L = 5]$ biased first-order Integrated Differential Approximant [35].

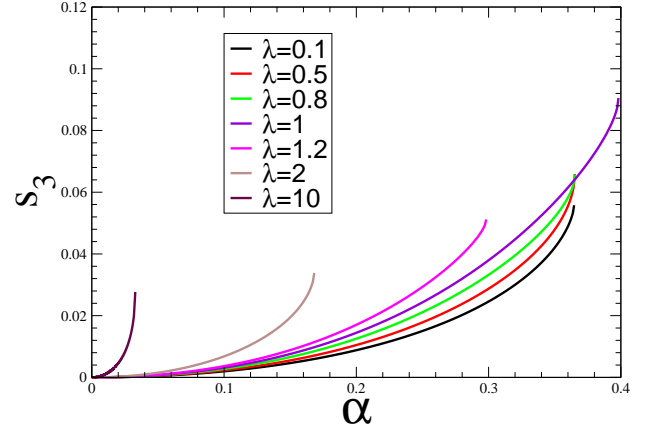


FIG. 5: Plots of the ‘Area-law’ or entanglement entropy per unit boundary length for the third Renyi entropy S_3 .

Renyi entropy a comparison with recent Quantum Monte Carlo study[34] is also made. The overall agreement is very good. Results from series expansion should be much more accurate away from the critical point.

The quantity of primary interest in our study is the corner entropy and its singular behavior. On approach to the critical coupling, we expect the corner entropy to

behave as

$$c_n = a_n \ln \xi = -\nu a_n \ln(\alpha_c - \alpha). \quad (4)$$

Here a_n should be a universal constant equal to the coefficient in the logarithmic size dependence $a_n \ln L$ of the entanglement entropy for a square region of linear dimension L when the system is right at the critical coupling[14, 26].

To analyze the corner entropy, we first take a derivative of the series, which converts a logarithmic singularity into a simple pole. We then study this by a simple Pade approximant biasing the critical point to that obtained from the analysis of the susceptibility series. The estimated a_n values are shown in Figure 6. In the Ising limit, our results are in excellent agreement with previous series expansions[24] and Numerical Linked Cluster (NLC) calculations[25] for the transverse-field Ising model. Very near the Heisenberg point, one expects greater uncertainty in the values due to crossover effects. Hence, we consider the values at $\lambda = 2$ and $\lambda = 10$. At $\lambda = 2$ we estimate $a_2 = -0.0055 \pm 0.0003$ while at $\lambda = 10$ we estimate $a_2 = -0.0059 \pm 0.0005$. These values agree well with the transverse field Ising model values of -0.0055 ± 0.0005 from series expansions[24, 38] and -0.0053 from the NLC calculations[25]. Quantum Monte Carlo estimates so far have[39] much larger error bars -0.0075 ± 0.0025 , but are also consistent with these estimates. For the third Renyi entropy, we estimate $a_3 = -0.0040 \pm 0.0003$ at $\lambda = 2$ and $a_3 = -0.0042 \pm 0.0004$ at $\lambda = 10$. These values are also in excellent agreement with the transverse-field Ising model values calculated by NLC. These results point strongly towards the universality of these coefficients in the Ising phase of this model and also between this model and the transverse-field Ising model.

We are not aware of any previous calculations of log singularities for the XY universality class. Our results lead to estimates of $a_2 = -0.0125 \pm 0.0006$ at $\lambda = 0.2$ and $a_2 = -0.0127 \pm 0.0013$ at $\lambda = 0.5$. Similar results for the third Renyi entropy are $a_3 = -0.0089 \pm 0.0006$ at $\lambda = 0.2$ and $a_3 = -0.0091 \pm 0.0020$ at $\lambda = 0.5$. These results clearly point towards a universal value for this universality class also.

At the Heisenberg point ($\lambda = 1$) our results have greater uncertainty. In the Fig. 6, the a_n values are shown for the critical point biased at $\alpha_c = 0.3982$ (estimate from susceptibility series), which leads to $a_2 = -0.023 \pm 0.005$ and $a_3 = -0.016 \pm 0.005$. If we bias the critical point to $\alpha_c = 0.3965107$ known more accurately from previous studies[31], we get $a_2 = -0.022 \pm 0.005$ and $a_3 = -0.016 \pm 0.005$. Corner entanglement entropy of this model has been studied before using NLC[26] and QMC[34]. The NLC values were found to be very close to 3 times the transverse-field Ising model values for all Renyi indices. Also, the QMC fits gave $a_2 = -0.016 \pm 0.001$. Our numbers are somewhat larger than these but still in fair agreement with them. Overall,

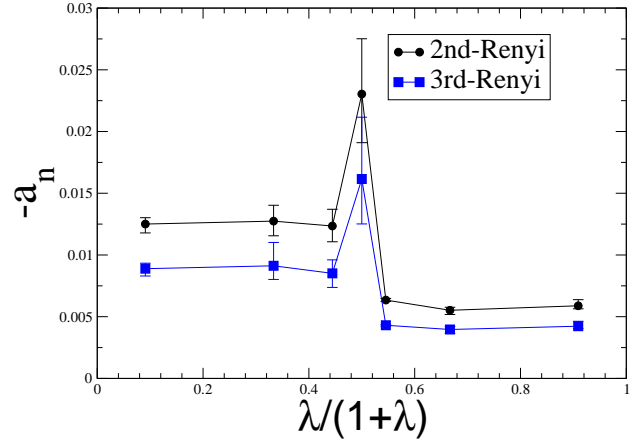


FIG. 6: Coefficient $-a_n$ of the logarithmic singularity associated with a corner in the boundary. These results show that the Ising and XY universality classes have constant coefficients. At Heisenberg symmetry the coefficient is largest. Our results are consistent with a rough proportionality for the log coefficients with the number of gapless modes in the system.

it is clear that the results imply a rough proportionality between the singular coefficients and the number of soft modes in the system that become gapless at the critical point.

In conclusion, in this paper we have studied a bilayer XXZ model that allows us to tune between Ising, Heisenberg and XY universality classes. We have calculated the ‘area-law’ terms and corner entanglement Renyi entropies using series expansion. We presented strong evidence that the corner entanglement has a logarithmic singularity, which takes universal values in different universality classes. Furthermore, this universal coefficient is roughly proportional to the number of soft or gapless modes in the system. Within these models, its magnitude decreases monotonically from less stable to more stable fixed points. However, the question of whether it is truly monotonic under renormalization and can serve the purpose of organizing stability of higher dimensional fixed points of quantum statistical models, analogous to the central charge c in one-dimensional models, deserves further attention.

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